

LA-UR-02-5840

Approved for public release;
distribution is unlimited.

Title: SECOND-ORDER, LOCAL BOUND-PRESERVING,
REMAPPING FOR ALE METHODS

Author(s): Mikhail Shashkov, T-7, 115213
Milan Kurcharick, T-7, 173031
Burton Wendroff, T-7, 053836

Submitted to: Second M.I.T. Conf. on Comp. Fluid and Solid Methods
June 17-20, 2003
Massachusetts Institute of Technology
Cambridge, MA 02139



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Form 836 (8/00)

Second-Order, Local-Bound-Preserving, Remapping for ALE Methods

Milan Kuchařík¹ Mikhail Shashkov² Burton Wendroff²

Abstract

In this paper we describe an efficient, second-order accurate, local-bound-preserving remapping (conservative interpolation) algorithm for Arbitrary Lagrangian-Eulerian (ALE) methods. The algorithm is based on reconstruction, approximate integration and mass redistribution.

Key words: ALE Methods; Conservative Interpolation; Remapping

1 Introduction

Consider that we have a mesh that is a tessellation of some region Ω by a collection of cells C_i $i = 1, \dots, L$, that is, the cells have disjoint connected interiors and their union is Ω . This we will call the old mesh.

Next, suppose there is a new tessellation of the region with a different collection

¹ Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University

in Prague, Břehová 7, 115 19 Prague 1, Czech Republic

² Group T-7, Los Alamos National Laboratory, Los Alamos, NM 87544, USA

of cells \tilde{C}_i $i = 1, \dots, L$, such that each new cell \tilde{C}_i is obtained by a small displacement of the vertices of the old cell C_i .

In the context of ALE methods the old mesh would be the result of the Lagrangian step and the new mesh would be the result of mesh modification (rezoning).

The situation is that the only data that the computation has at hand are, for each cell C_i , the mass for some density function $\rho(\mathbf{x})$, said mass being

$$m_i = \int_{C_i} \rho(\mathbf{x}) dV,$$

with corresponding mean value

$$\bar{\rho}_i = \frac{m_i}{V(C_i)},$$

where $V(C_i)$ is the volume of C_i .

The conservative interpolation (remapping) problem is to compute the masses \tilde{m}_i and mean values of the new grid, but since the density distribution is unknown we can only approximate them. We will denote these approximate values by \tilde{m}_i^* . This approximation has to be exact for a global linear function and total mass should be conserved.

A possible procedure for accomplishing this has two stages. First, one constructs a new distribution $\hat{\rho}(x)$ such that $\int_{C_i} \hat{\rho}(\mathbf{x}) dV = m_i$ and, if $\rho(\mathbf{x})$ is a global linear function then $\hat{\rho}(\mathbf{x}) \equiv \rho(\mathbf{x})$ - the reconstruction step. In this paper

we use the Barth-Jaspersen limiting procedure to construct a piece-wise linear function $\hat{\rho}(\mathbf{x})$ (see, for example, [1]). It guaranties that the value of $\hat{\rho}(\mathbf{x})$ at cell \tilde{C}_i is within local bounds as defined by the maximum and minimum of mean values in cell C_i and its nearest neighbors.

For the second stage $\hat{\rho}(\mathbf{x})$ is *exactly* integrated over the new cells. This requires finding the intersection of each new cell with the old ones. It is doable but computationally very expensive in two dimensions, but not feasible in three dimensions. We will call such a method "exact" and use it as the reference method.

In this paper we present a new efficient, conservative, local-bound-preserving, second-order accurate algorithm which does not require finding intersections.

The first stage of our new method is the same as for the exact method.

In the second stage, the new mass is written in flux form (which guaranties conservation of total mass), that is, the mass of each new cell will be set to the mass of the corresponding old cell plus fluxes which define the exchange of mass with nearest neighbors. These fluxes are computed by using a quadrature, which does not require finding the intersections.

It may happen (because of approximate integration) that the new means will be out of local bounds, for example, they can be negative even if the old means were all positive.

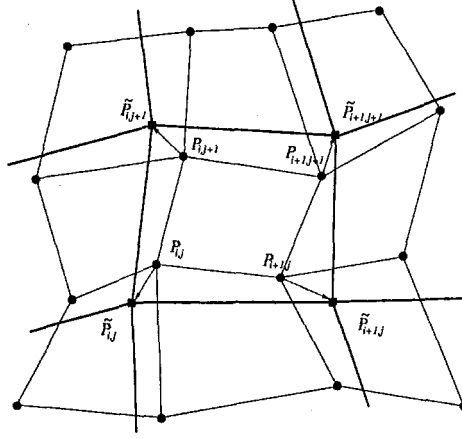


Fig. 1. Old (thin lines and solid circles) and New mesh (bold lines and solid squares); Swept regions.

To fix out of bound means we introduce a third stage, wherein masses of new cells are redistributed in such a way that modified new means are in the range of local bounds.

In the following sections we will describe the algorithm and give some numerical examples.

2 Remapping Algorithm

The method we are describing is by no means restricted to a logically rectangular grid or to 2D, but we explain it in those terms.

The vertices of a logically rectangular grid are $P_{i,j} = (x_{i,j}, y_{i,j})$, $i = 1, \dots, m$, $j = 1, \dots, n$. The cells $C_{i+\frac{1}{2},j+\frac{1}{2}}$ are the quadrilaterals formed by the four vertices $P_{i,j}$, $P_{i+1,j}$, $P_{i+1,j+1}$, $P_{i,j+1}$ (see Fig. 1).

2.1 Approximate Integration

The approximate new mass $\tilde{m}_{i+\frac{1}{2},j+\frac{1}{2}}^*$ is defined in terms of the old mass $m_{i+\frac{1}{2},j+\frac{1}{2}}$, and mass exchange with neighboring cells,

$$\tilde{m}_{i+\frac{1}{2},j+\frac{1}{2}}^* = m_{i+\frac{1}{2},j+\frac{1}{2}} + \mathcal{F}_{i+1,j+\frac{1}{2}} - \mathcal{F}_{i,j+\frac{1}{2}} + \mathcal{F}_{i+\frac{1}{2},j+1} - \mathcal{F}_{i+\frac{1}{2},j}. \quad (1)$$

Here \mathcal{F} are edge fluxes, which are defined following ideas from [1] and will be described next.

Consider an edge $F_{i,j+\frac{1}{2}} = \{P_{i,j}, P_{i,j+1}\}$. This edge is common to cells $C_{i+\frac{1}{2},j+\frac{1}{2}}$ and $C_{i+\frac{3}{2},j+\frac{1}{2}}$. Rezoning moves $P_{i,j}$ to its new position $\tilde{P}_{i,j}$ and $P_{i,j+1}$ to $\tilde{P}_{i,j+1}$, thereby forming a quadrilateral $\delta F_{i,j+\frac{1}{2}} = (P_{i,j}, \tilde{P}_{i,j}, \tilde{P}_{i,j+1}, P_{i,j+1})$ (see Fig. 1), which we will call the swept region.

The critical function of the swept region is its *signed* area $V(\delta F_{i,j+\frac{1}{2}})$, which sign depends on the ordering of its vertices. It is introduced by expressing the area in terms of a line integral as follows:

$$V(\delta F_{i,j+\frac{1}{2}}) = \int_{\delta F_{i,j+\frac{1}{2}}} dV = \oint_{\partial(\delta F_{i,j+\frac{1}{2}})} x dy. \quad (2)$$

For situation shown in Fig. 1, $V(\delta F_{i,j+\frac{1}{2}}) < 0$.

We can introduce *signed* (see, [1]) integration of any polynomial function over a polygon by reducing it to a line integral similar to (2). In the rest of the paper we will understand all integrals in this sense.

We define the flux $\mathcal{F}_{i,j+1/2}$ in (1) as follows

$$\mathcal{F}_{i,j+\frac{1}{2}} = \int_{\delta(F_{i,j+\frac{1}{2}})} \hat{\rho}_{i,j+\frac{1}{2}}(x, y) dV,$$

where

$$\hat{\rho}_{i,j+\frac{1}{2}}(x, y) = \begin{cases} \hat{\rho}_{i+\frac{1}{2},j+\frac{1}{2}}(x, y), & V(\delta F_{i,j+\frac{1}{2}}) \geq 0, \\ \hat{\rho}_{i-\frac{1}{2},j+\frac{1}{2}}(x, y), & V(\delta F_{i,j+\frac{1}{2}}) < 0. \end{cases}$$

In words, in the swept region the integrand is taken entirely from the cell on one side or the other of the edge, depending on the sign of the swept area. For example, in the case shown in Fig. 1 $V(\delta F_{i,j+\frac{1}{2}}) < 0$ and we use the reconstructed linear function belonging to the left side of the edge ($\tilde{\rho}_{i-\frac{1}{2},j+\frac{1}{2}}(x, y)$) because most of the swept region lies inside cell $C_{i-\frac{1}{2},j+\frac{1}{2}}$.

2.2 Conservative Mass Re-Distribution

The quantity which one is remapping may have specific physical meaning. For example, the given means might be derived from a concentration lying between zero and one, and for the remapped means to be physically correct they have to be in the same range. At this point our algorithm may create values out of range, especially for non-smooth ρ . Here we describe a procedure based on mass redistribution which locally adjusts the out of range values to be within the bounds.

By way of illustration, suppose all the initial means are nonnegative and that we would like the same to be true of the remapped means. Now, suppose that the mass of some new cell $\tilde{C}_{i+\frac{1}{2},j+\frac{1}{2}}$, computed using (1), is negative. Let $m^- = \tilde{m}_{i+\frac{1}{2},j+\frac{1}{2}}^* < 0$. We look at the eight immediate neighbors of the cell and compute the total mass M of those neighbors having positive masses. If $M \geq |m^-|$, we can reduce each of those positive masses m^+ by $m^+ |m^-|/M$, and then set $\tilde{m}_{i+\frac{1}{2},j+\frac{1}{2}}^* = 0$, thereby conserving mass. If $M < |m^-|$ then we cannot correct the negative mass from the eight neighbors. In this case one can try larger neighborhoods. Eventually by extending neighborhoods we will be able to correct negative value because total mass is conserved and is positive. However, in all examples which we have run it was enough to use only nearest neighbors.

A similar procedure can be done for any global or local bound. For example, we could take as upper and lower bounds the maximum and minimum of neighboring old cell values. In fact, in the numerical examples presented in the next section such local bounds were imposed.

3 Tests

In this section we compare our new method and the exact method.

Here we assume that we have a sequence of grids $\{x_{i,j}^n, n = 0, \dots, n_{max}\}$, the superscript identifying a particular grid. We begin with a given test function

$\rho(x, y)$ and compute its means on grid $x_{i,j}^0$, then remap the function means from grid $x_{i,j}^0$ to grid $x_{i,j}^1$, and then remap resulting means from grid $x_{i,j}^1$ to grid $x_{i,j}^2$, etc. This allows us to look at the cumulative effect of many remappings.

In our experiments we will use a sequence of 100 *random* grids, where each grid is obtained by random perturbation of the uniform grid in unit square (see [1]).

We will use smooth *Sine* test function $\rho(x, y) = 1 + \sin(2\pi x) \sin(2\pi y)$, and discontinuous *Square* test function, the later being equal to one in a small square centered in $(0.5, 0.5)$ with side equal to 0.173 and zero in the rest of the domain.

3.1 Numerical Experiments

First, we remap the sine test function. The results of the computations demonstrate second-order convergence in the discrete L_1 and max norms for both methods. The errors for both methods are very close.

Second, we remap the square test function. Here we use the 50^2 grid. The L_1 norms of the errors are 3.07^{-2} and 2.95^{-2} for exact and new method respectively. The max norm errors are 6.64^{-1} and 6.60^{-1} . Final isolines are presented in Fig. 2. Visually the isolines are almost indistinguishable.

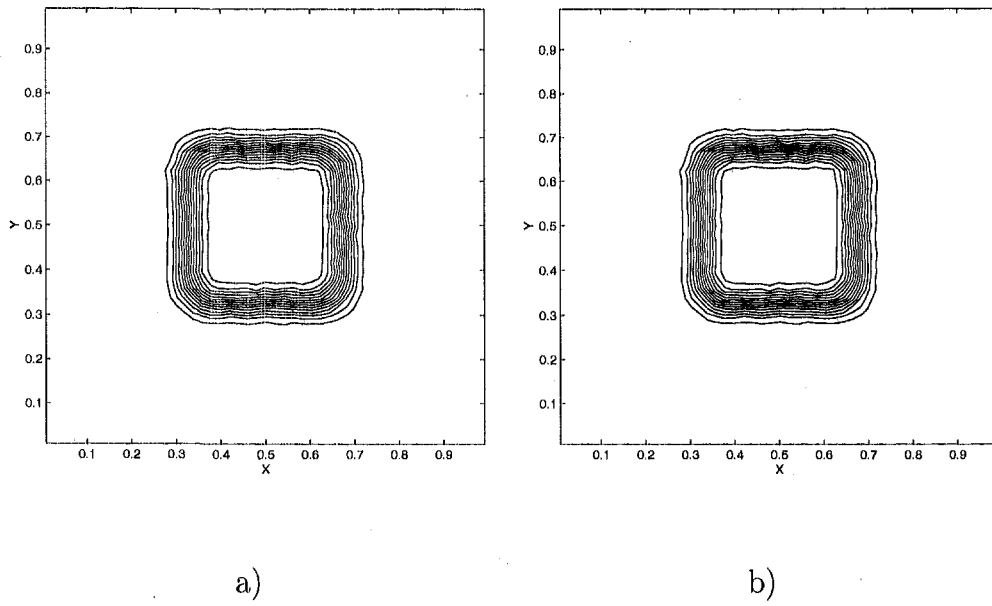


Fig. 2. Isolines for remapping of square test function: a) Exact method, b) New method.

References

- [1] L. Margolin and M. Shashkov, *Second-order sign-preserving remapping on general grids*, Technical Report LA-UR-02-525, Los Alamos National Laboratory, 2002, (<http://cnls.lanl.gov/~shashkov>), Submitted to Journal of Computational Physics.